phenol, 4,4'-butylidenebis-4731-84-4 | DTXSID20280701

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.85

Global applicability domain: Inside

Local applicability domain index: 5.02e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

Image not found
Diethylstilbestrol
Measured: 5.07
Predicted: 3.98

Image not found
Bisphenol A
Measured: 3.32
Predicted: 3.20